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Light focusing by silicon nanosphere structures under conditions of magnetic dipole and quadrupole resonances

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Abstract. Metalens is a planar device for light focusing. In this work, we design and optimize c-Si nanosphere metalenses working on the magnetic dipole and quadrupole resonances of the c-Si nanoparticle. Resonant optical response of c-Si nanostructures is simulated by the multipole decomposition method along with the zero-order Born approximation. Limitations of this approach are investigated. The obtained results of optimization are verified by simulation via the T-matrix method.

1. Introduction

The structures of many subwavelength particles for light focusing, namely metalenses, are considered by researchers as the perspective elements for future optical devices [1, 2]. However, to design widely-functional metalenses with the desired characteristics, advanced optimization techniques are needed [2, 3]. In this case, speed and efficiency of optimization are determined by a physical model describing a collective response of metalens elements, typically arranged in rings. In this work, we consider metalenses composed of c-Si nanosphere rings. We suggest the model when the optical response of the nanoparticle is associated with several multipoles while the collective response of nanoparticles structure is described in the zero-order Born approximation [4]. We find the limitations of our approach and apply an evolutionary algorithm [5] for optimization of ultra-thin Si nanosphere metalenses working at the magnetic dipole and quadrupole resonances of the nanoparticle [6, 7]. The accuracy of the results obtained in the Born approximation is verified by comparison with the rigorous T-matrix method [8].

2. Results and Discussion

We consider the structures consisting of N c-Si nanospheres with a diameter of 200 nm. According to Fig. 1(a), the optical response of single particle can be associated with the dipoles and quadrupoles of electric and magnetic types. The interaction of multipoles corresponding to the different nanoparticles can be taken into account under the coupled multipole model (see Eq. (25) in [11]):

$$\mathbf{Y} = \mathbf{Y}_0 + \hat{\mathbf{V}}\mathbf{Y}, \quad (1)$$



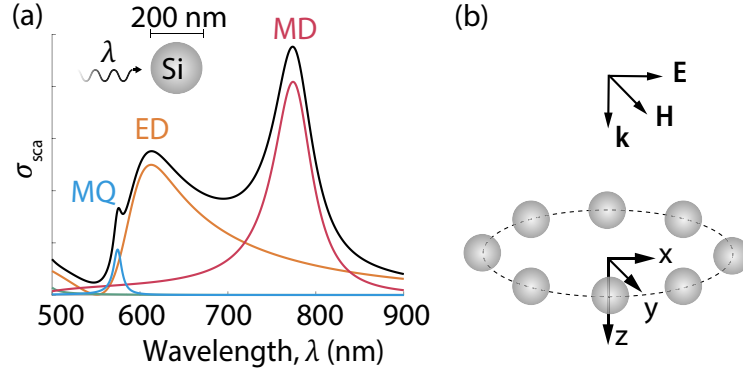


Figure 1. (a) Scattering spectrum of a silicon nanosphere having a diameter of 200 nm calculated from the Mie-theory [9]. Red, orange, blue, and green lines correspond to the MD, ED, MQ, and EQ contributions, respectively. Dispersion of c-Si is taken into account [10]. (b) Schematic view of a single nanosphere ring with the shown incident wave and Cartesian coordinates system.

where \mathbf{Y} is the vector of self-consistent multipole moments:

$$\mathbf{Y} = [p_x^1, \dots, p_z^N, m_x^1, \dots, m_z^N, Q_{xx}^1, \dots, Q_{zz}^N, M_{xx}^1, \dots, M_{zz}^N]_{24N}^T, \quad (2)$$

\mathbf{Y}_0 is the vector of moments excited only by the incident wave:

$$\mathbf{Y}_0 = [p_{0,x}^1, \dots, p_{0,z}^N, m_{0,x}^1, \dots, m_{0,z}^N, Q_{0,xx}^1, \dots, Q_{0,zz}^N, M_{0,xx}^1, \dots, M_{0,zz}^N]_{24N}^T, \quad (3)$$

$\hat{\mathbf{V}}$ is the $24N \times 24N$ interaction matrix composed of Green's tensors blocks.

Solving Eq. (1), we can find the self-consistent multipole moments of nanoparticles:

$$\mathbf{Y} = (\hat{\mathbf{U}} - \hat{\mathbf{V}})^{-1} \mathbf{Y}_0, \quad (4)$$

if $\det(\hat{\mathbf{U}} - \hat{\mathbf{V}}) \neq 0$, where \mathbf{U} is the $24N \times 24N$ unity matrix. If the electromagnetic coupling between particles is weak enough, it can be neglected, which corresponds to the zero-order Born approximation (ZBA). The ZBA multipole moments of nanoparticles

$$\mathbf{Y} = \mathbf{Y}_0 \quad (5)$$

connect with the incident fields \mathbf{E}_0 and \mathbf{H}_0 through the Mie-polarizabilities [11]:

$$\mathbf{p}_0^j = \alpha_p \mathbf{E}_0(\mathbf{r}_j), \quad (6)$$

$$\mathbf{m}_0^j = \alpha_m \mathbf{H}_0(\mathbf{r}_j), \quad (7)$$

$$\hat{Q}_0^j = (\alpha_Q/2) [\nabla \mathbf{E}_0(\mathbf{r}_j) + \mathbf{E}_0(\mathbf{r}_j) \nabla], \quad (8)$$

$$\hat{M}_0^j = (\alpha_M/2) [\nabla \mathbf{H}_0(\mathbf{r}_j) + \mathbf{H}_0(\mathbf{r}_j) \nabla], \quad (9)$$

Knowing the multipole moments, we can calculate the total electric \mathbf{E} and magnetic \mathbf{H} fields in the system (using Eqs. (13)-(16) from [11]), and the electromagnetic intensity $I(\mathbf{r})/I_0 = (|\mathbf{E}(\mathbf{r})|^2 + Z^2 |\mathbf{H}(\mathbf{r})|^2) / 2E_0^2$ where \mathbf{r} is the observation point, Z is the free-space impedance, E_0 is the amplitude of electric field in the incident plane wave.

Using the ZBA, we study light focusing by a single ring of Si nanospheres shown in Fig. 1(b). Due to the axial symmetry, the ring has a focus on its axis (here z -axis). Hence, ring focal

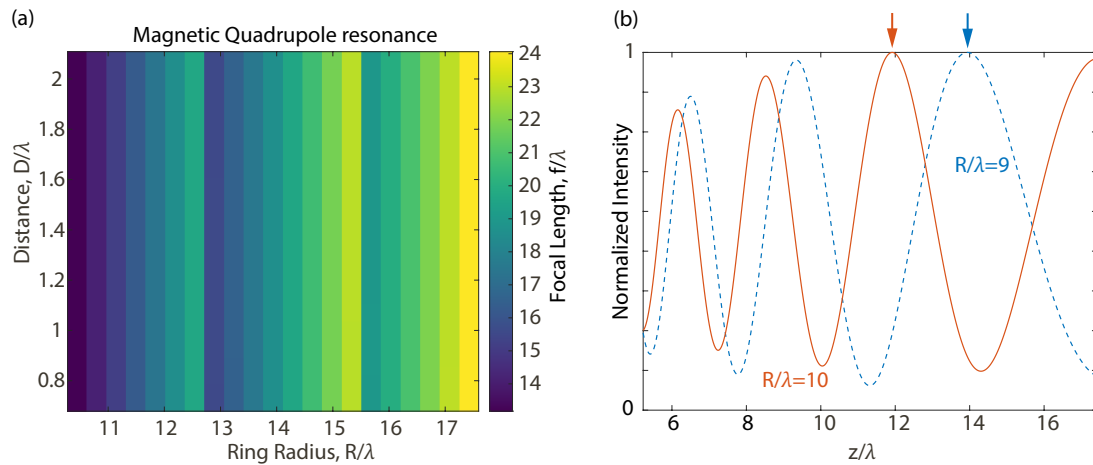


Figure 2. Features of light focusing at the MQ resonance $\lambda = 574$ nm. (a) Focal length of single nanosphere ring as a function of the ring radius and center-center distance between particles. (b) Normalized (on the maximum) electromagnetic intensity distribution along the z -axis for the ring radius $R/\lambda = 9$ (blue dashed line) and $R/\lambda = 10$ (red solid line). The number of particles in both rings $N = 32$. The arrows indicate the focal lengths of rings. The results are obtained in the ZBA.

length is defined as the distance between the ring plane and the position of the highest intensity peak on the ring axis. Dependence of the ring focal length on the ring parameters for the MQ resonance is shown in Fig. 2(a). The ring focal length is almost completely determined by its size. Moreover, this dependence is non-monotonic due to the interference origin of the intensity peaks. As a result of constructive interference between the incident wave and the scattered waves, the bigger ring may have a shorter focal length [see focal lengths in Fig. 2(b)]. Similar behavior of the focal length is observed at the MD resonance.

The focal length and focal intensity are the basic parameters of metalens. The error of calculating these quantities in the ZBA was studied for the single ring at the MD and MQ resonances. This error was defined as follows: $\Delta(V) = 100\% \times |V^{\text{CMM}} - V^{\text{ZBA}}|/V^{\text{CMM}}$, where V^{CMM} and V^{ZBA} are values of V calculated using moments (4) and (5), respectively. We calculate errors of the ring focal length $\Delta(f)$ and intensity $\Delta(I)$ as functions of ring radius $6 \mu\text{m} \leq R \leq 10 \mu\text{m}$ and distance between centers of particles $200 \text{ nm} \leq D \leq 1200 \text{ nm}$. We obtain that the focal length error $\Delta(f) \leq 2.5\%$ at the both resonances for all ring parameters; the focal intensity error $\Delta(I) \lesssim 10\%$ when the inter-particle distance $D \geq 0.66\lambda$ and $D \geq 0.92\lambda$ at the MQ and MD resonances, respectively. We will call these distance values limiting. Hence, to simulate Si nanosphere metalenses via the ZBA-based approach, the inter-particle distance should be higher than limiting.

Based on the ZBA calculation scheme is directly comparable with the optimization algorithm. To optimize metalenses, we choose an evolutionary SEMO algorithm [5]. We use this algorithm to optimize metalenses at the MQ and MD resonances. The objective functions of optimization are both desired focal length (here $f = 5 \mu\text{m}$) and high focal intensity. During the optimization, the algorithm varies the number of rings, their radii, and the number of particles in the ring. The fixed parameters: diameter of Si nanoparticle is 200 nm, metalens size to 20 μm , minimal inter-particle distance is equal to $1.11\lambda_{\text{MQ}}$ and $1.07\lambda_{\text{MD}}$. The optimized metalenses with $f = 5 \mu\text{m}$ and their intensity profiles are shown in Fig. 3.

We compare intensity profiles, obtained in ZBA, with the ones calculated by the T-matrix method [8] and obtain a good agreement. Both methods determine the same focal length equalled

to $5 \mu\text{m}$ and $4.9 \mu\text{m}$ for MQ and MD resonances, while the error of focal intensity: 5.7% and 3%, respectively.

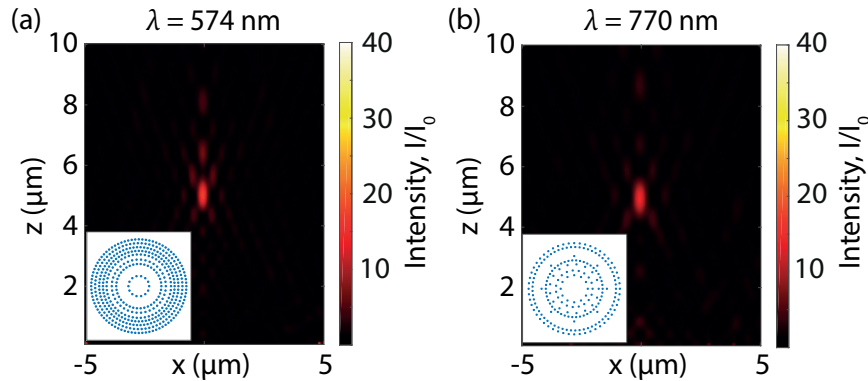


Figure 3. Normalized electromagnetic intensity distribution in the xz -plane for metalenses optimized at the MQ (a) and MD (b) resonances (I_0 is the intensity of incident wave). Both metalenses have the focal length $f = 5 \mu\text{m}$. In insets: distribution of nanoparticles in the xy -plane for optimized metalenses. The results are obtained in the ZBA.

3. Conclusion

We studied light focusing by c-Si nanosphere rings. The optical response of such structures was described using the dipole-quadrupole model along with the zero-order Born approximation. We showed that this approach provides a low-error simulation of the resonant optical response if the distance between particles $\gtrsim \lambda_0$. We optimized positions of Si nanospheres, using an evolutionary algorithm, and obtained effective metalenses with the desired focal lengths, working at the magnetic dipole and quadrupole resonances of the single nanosphere. The results of optimization in ZBA demonstrate a good agreement with the T-matrix method simulation.

4. Acknowledgments

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